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Towards real-space mapping of valence states using core-loss EFTEM imaging

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Thanks to the improvements in aberration-correction for electron microscopes, it is now possible to determine the position and species of individual atom columns with high accuracy. In particular cases, one can even resolve details at a sub-atomic level, like effects of the electron redistribution in the vicinity of a defect due to chemical bonding [1]. On the other hand, electron energy-loss spectroscopy (EELS) is a powerful method to investigate electronic excitations like plasmons (valence-loss) and interband transitions (core-loss region). In particular, near-edge spectra contain valuable information on conduction states and chemical (anti)binding.

This raises the question, if it is possible to map individual atomic orbitals in real space by combining the spatial resolution of transmission electron microscopes (TEM) with the analytical power of electron energy-loss spectroscopy. At the atomic level, a detailed understanding of the imaging process is only possible in the framework of quantum mechanics and, in order to extract information from the recorded images, a detailed comparison with image simulations is mandatory. Indeed, previous calculations including elastic and inelastic scattering [2] predict the possibility to map the orientation of selected anti-binding states in real-space using EFTEM imaging (energy-filtered transmission electron microscopy) at high energy loss.

In order to evaluate the feasibility of corresponding experiments, we have performed EFTEM imaging for two different samples, Silicon and Rutile (TiO_2). We show that lattice planes can be resolved in core-loss EFTEM and we assess the importance of image aberrations, signal-to-noise, and other limiting factors for orbital mapping. Due to the small scattering cross section for high energy-loss the image intensity is very low. Single recorded images have no apparent structure and the periodicity of the crystal is only clearly visible in the FFT (see Figure 1). We propose an averaging method to improve the S/N ratio of the high-resolution images by making use of the translational symmetry of the crystal summing over many neighbouring unit-cells.

1. J.C. Meyer *et.al.*, Nature Materials, 10 (2011), p. 209.
2. S. Löffler, V. Motsch and P. Schattschneider, submitted to Ultramicroscopy.
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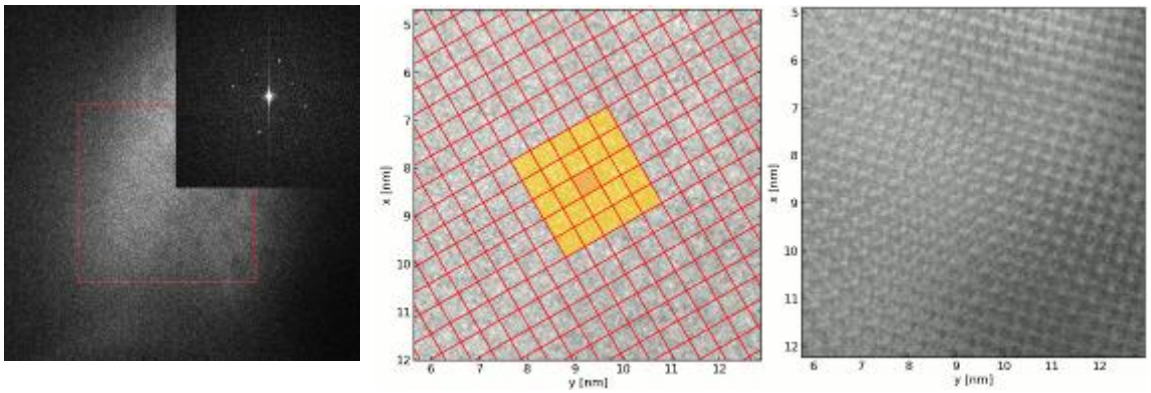

(a) (b) (c)

Figure 1. a) Energy-loss filtered HRTEM image of Rutile at the Ti-L edge (E=463eV, dE=2eV). The inset shows the modulus of the FFT of the highlighted region. The inhomogeneous illumination is due to the strong convergence of the beam. b) Superposition of crystal periodicity and the central part of the HRTEM image (red lines). c) The summed image resulting from a running average over 5x5 unit cells (indicated in yellow) shows atom contrast.